

Nuclear spin-lattice relaxation rate in noncentrosymmetric superconductor Y_2C_3

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Abstract

For a noncentrosymmetric superconductor such as Y_2C_3 , we consider a parity-mixing model composed of spin-singlet s -wave and spin-triplet f -wave pairing components. The d -vector in f -wave state is chosen to be parallel to the Dresselhaus asymmetric spin-orbit coupling vector. It is found that, the quasiparticle excitation spectrum exhibits distinct nodal structure as a consequence of parity-mixing. Our calculation predict anomalous noninteger power laws for low-temperature nuclear spin-lattice relaxation rate T_1^{-1} . We demonstrate particularly that such a model can qualitatively account for the existing experimental results of the temperature dependence of T_1^{-1} in Y_2C_3 .

Keywords: Noncentrosymmetric superconductor Y_2C_3 , Pairing symmetry, Nuclear spin-lattice relaxation rate

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1. Introduction

The physics of unconventional superconductivity in materials without inversion symmetry has become a subject of growing interest [1, 2] since the noncentrosymmetric (NCS) heavy Fermion superconductor CePt_3Si was found in 2004 [3]. In these materials the superconducting phase develops in a low-symmetry environment with a missing inversion center. This broken symmetry generates

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an antisymmetric spin-orbit (SO) coupling and prevent the usual even/odd classification of Cooper pairs according to orbital parity, allowing a mixed-parity superconducting state [4, 5]. This mixture of the pairing channels with different parities may result in unusual temperature and field dependence of experimentally observed superconducting properties [1, 2].

For CePt₃Si, in particular, where the Rashba-type [6] SO coupling vector $\gamma_{\mathbf{k}} \propto (\hat{k}_y, -\hat{k}_x, 0)$ is generated, various low-energy thermodynamical and transport properties have been extensively investigated from both the experimental and theoretical sides. The NMR relaxation rate [7] T_1^{-1} , thermal conductivity [8], and London penetration depth [9] indicate power law behavior at lowest temperatures, suggesting the presence of nodal lines in the quasiparticle excitation spectrum. Besides, the upper critical magnetic field H_{c2} is surprisingly large [3, 10], and no change in the Knight shift across the transition temperature T_c [11] has been observed. These characteristics are attributed to a spin triplet superconducting order parameter. Theoretically, Frigeri *et al.* have proposed an $(s+p)$ -wave model [12] where the d -vector of p -wave state is chosen to be parallel to the SO coupling vector ($\mathbf{d}_{\mathbf{k}} \propto \mathbf{g}_{\mathbf{k}}$). The gap function of this $(s+p)$ -wave model has the natural form for a system without inversion symmetry, and exhibits line nodes when the p -wave pair potential is larger than that of s -wave one. It should be noted that a nonzero s -wave pair potential is necessary to get expected line nodes. Hayashi *et al.* [13] have demonstrated that the presence of line nodes in this $(s+p)$ -wave model may account for the experimentally observed low-temperature features of the nuclear spin-lattice relaxation rate T_1^{-1} in CePt₃Si on a qualitative level.

The cubic Pu₂C₃-type sesquicarbide compound Y₂C₃ is a NCS superconductor known for its relatively high superconducting transition temperature [14] ($T_c \sim 18\text{K}$). Different from the CePt₃Si case, the Dresselhaus [15] SO coupling vector $\gamma_{\mathbf{k}} \propto (\hat{k}_x(\hat{k}_y^2 - \hat{k}_z^2), \hat{k}_y(\hat{k}_z^2 - \hat{k}_x^2), \hat{k}_z(\hat{k}_x^2 - \hat{k}_y^2))$ is relevant to Y₂C₃.

Even many years after its discovery, the nature and symmetry of the superconducting gap function in Y₂C₃ appears to be full of contradiction. While the specific heat measurement [16] and tunneling experiment [17] are interpreted as

a fully gapped isotropic s -wave state, the nuclear spin-lattice relaxation rate [18] T_1^{-1} and muon spin rotation [19] (μ SR) measurements on Y_2C_3 are qualitatively fitted with a nodeless two-gap model similar to MgB_2 . On the other hand, Chen *et al.* [20] have measured the magnetic penetration depth as a function of temperature and found a weak linear dependence at very low temperatures. They also reanalysed the NMR data reported in Ref. [18] and claimed that, where $T_1^{-1} \sim T^3$ at $T < 3\text{K}$, as a matter of fact. Such behavior seems to support the existence of line nodes rather than a fully opened gap in the superconducting state of Y_2C_3 . In addition, the upper critical magnetic field H_{c2} is found to be compatible with the paramagnetic limiting field [10, 20], and the Knight shift in NMR [18] is decreased to approximately 2/3 of its normal-state value. These features are again incompatible with the single gap or two-gap s -wave pictures. It is expected that line nodes (or point nodes of second-order) would be generated due to parity-mixing, similar to the case of CePt_3Si mentioned above. In order to shed light on these controversy, further experimental and theoretical studies on the superconducting properties of Y_2C_3 are required.

In this work, we theoretically investigate the nuclear spin-lattice relaxation rate [18] T_1^{-1} on the basis of $(s+f)$ -wave model, where the d -vector in f -wave state is chosen to be parallel to the Dresselhaus-type asymmetric SO coupling vector. We analyse various possible nodal structures which can be generated by the effect of parity-mixing. In particular, the temperature dependence of the nuclear spin-lattice relaxation rate T_1^{-1} is calculated and compared with the experimental result obtained in Ref. [18] for Y_2C_3 .

2. Model Hamiltonian

Our starting point is the following mean-field $(s+f)$ -wave pairing Hamiltonian

$$H = H_0 + H_{int}. \quad (1)$$

The Hamiltonian H_0 describes the noninteracting conduction electrons in a NCS crystal,

$$H_0 = \sum_{\mathbf{k}} \sum_{\alpha, \beta} (\epsilon_{\mathbf{k}} \sigma_0 + \gamma_0 \boldsymbol{\gamma}_{\mathbf{k}} \cdot \boldsymbol{\sigma})_{\alpha\beta} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}\beta}, \quad (2)$$

where $c_{\mathbf{k}\alpha}^\dagger$ ($c_{\mathbf{k}\alpha}$) creates (annihilates) an electron with wave vector \mathbf{k} and spin α , $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ denotes the vector of Pauli matrices, σ_0 is the 2×2 unit matrix, $\epsilon_{\mathbf{k}}$ is the parabolic bare band dispersion measured relative to the chemical potential restricted to $|\epsilon_{\mathbf{k}}| < \omega_c$, with ω_c being the usual cutoff energy. Furthermore, $\boldsymbol{\gamma}_{\mathbf{k}} = (\hat{k}_x(\hat{k}_z^2 - \hat{k}_y^2), \hat{k}_y(\hat{k}_z^2 - \hat{k}_x^2), \hat{k}_z(\hat{k}_x^2 - \hat{k}_y^2))$, with $\hat{k}_x = \sin \theta_{\mathbf{k}} \cos \phi_{\mathbf{k}}$, $\hat{k}_y = \sin \theta_{\mathbf{k}} \sin \phi_{\mathbf{k}}$, and $\hat{k}_z = \cos \theta_{\mathbf{k}}$, is the asymmetric ($\boldsymbol{\gamma}_{\mathbf{k}} = -\boldsymbol{\gamma}_{-\mathbf{k}}$) Dresselhaus SO coupling vector considered to be relevant for Y_2C_3 and La_2C_3 . The strength of SO coupling is denoted by γ_0 .

The second term in Eq. (1) represents the pairing interaction:

$$H_{int} = \frac{1}{2} \sum_{\mathbf{k}} \sum_{\alpha, \beta} [\Delta_{\mathbf{k}, \alpha\beta} c_{\mathbf{k}\alpha}^\dagger c_{-\mathbf{k}\beta}^\dagger + \Delta_{\mathbf{k}, \alpha\beta}^\dagger c_{-\mathbf{k}\alpha} c_{\mathbf{k}\beta} + \Delta_{\mathbf{k}, \alpha\beta} F_{\mathbf{k}, \beta\alpha}^\dagger],$$

with the anomalous averages $F_{\mathbf{k}, \alpha\beta} = \langle c_{\mathbf{k}\alpha} c_{-\mathbf{k}\beta} \rangle$, and the gap function defined by [21]

$$\Delta_{\mathbf{k}, \alpha\beta} = - \sum_{\mathbf{k}'} \sum_{\lambda, \mu} V_{\beta\alpha, \lambda\mu}(\mathbf{k}, \mathbf{k}') F_{\mathbf{k}', \lambda\mu}, \quad (3)$$

where $V_{\alpha\beta, \lambda\mu}(\mathbf{k}, \mathbf{k}')$ is the pairing potential. In this work, we will adopt $V_{\alpha\beta, \lambda\mu}(\mathbf{k}, \mathbf{k}')$ as the phenomenological one [22]:

$$\begin{aligned} V_{\alpha\beta, \lambda\mu}(\mathbf{k}, \mathbf{k}') = & -\frac{V_s}{2} (i\sigma_y)_{\alpha\beta} (i\sigma_y)_{\lambda\mu}^\dagger - \frac{V_f}{2} (\boldsymbol{\gamma}_{\mathbf{k}} \cdot \boldsymbol{\sigma} i\sigma_y)_{\alpha\beta} (\boldsymbol{\gamma}_{\mathbf{k}'} \cdot \boldsymbol{\sigma} i\sigma_y)_{\lambda\mu}^\dagger \\ & + \frac{V_m}{2} [(\boldsymbol{\gamma}_{\mathbf{k}} \cdot \boldsymbol{\sigma} i\sigma_y)_{\alpha\beta} (i\sigma_y)_{\lambda\mu}^\dagger + (i\sigma_y)_{\alpha\beta} (\boldsymbol{\gamma}_{\mathbf{k}'} \cdot \boldsymbol{\sigma} i\sigma_y)_{\lambda\mu}^\dagger], \end{aligned} \quad (4)$$

where the first two terms represent the interaction in the s -wave pairing channel and in the spin-triplet f -wave pairing channel, respectively, and the last term describes the scattering between the two channels. In the following, we will

chose the interaction parameters V_s , V_f , and V_m to be positive, and take for simplicity $V_m = \sqrt{V_s V_f}$ which yields $\Delta_s(T)/\Delta_f(T) = \text{const.}$ [22].

Owing to the lack of inversion symmetry, the superconducting gap function Eq. (3) generally contains an admixture of even-parity spin-singlet and odd-parity spin-triplet pairing states,

$$\Delta_{\mathbf{k},\alpha\beta} = [\psi_{\mathbf{k}} i\sigma_y + \mathbf{d}_{\mathbf{k}} \cdot \boldsymbol{\sigma} i\sigma_y]_{\alpha\beta}, \quad (5)$$

where $\psi_{\mathbf{k}} = \psi_{-\mathbf{k}}$ and $\mathbf{d}_{\mathbf{k}} = -\mathbf{d}_{-\mathbf{k}}$ represent the spin-singlet and spin-triplet components, respectively. The direction of the $\mathbf{d}_{\mathbf{k}}$ (the d -vector) is assumed to be parallel to $\boldsymbol{\gamma}_{\mathbf{k}}$, as for this choice the antisymmetric SO interaction is not destructive for spin-triplet pairing[12]. Hence, we parametrize the \mathbf{d} -vector as $\mathbf{d}_{\mathbf{k}} = \Delta_f \boldsymbol{\gamma}_{\mathbf{k}}$. For the spin-singlet component we assume s -wave pairing $\psi_{\mathbf{k}} = \Delta_s$, and choose the amplitudes Δ_s and Δ_f to be real and positive.

Using the vector operator $\Psi_{\mathbf{k}} = (c_{\mathbf{k}\uparrow}, c_{\mathbf{k}\downarrow}, c_{-\mathbf{k}\uparrow}^\dagger, c_{-\mathbf{k}\downarrow}^\dagger)^t$, where $(\dots)^t$ stands for the transposing operation, we can write the Hamiltonian in a more compact form:

$$H = \frac{1}{2} \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \check{H}_{\mathbf{k}} \Psi_{\mathbf{k}} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k}} \sum_{\alpha,\beta} \Delta_{\mathbf{k},\alpha\beta} F_{\mathbf{k},\beta\alpha}^\dagger, \quad (6)$$

where

$$\check{H}_{\mathbf{k}} = \begin{pmatrix} \hat{M}_{\mathbf{k}} & \hat{\Delta}_{\mathbf{k}} \\ \hat{\Delta}_{\mathbf{k}}^\dagger & -\hat{M}_{-\mathbf{k}}^* \end{pmatrix}, \quad (7)$$

with

$$\begin{aligned} \hat{M}_{\mathbf{k}} &= \epsilon_{\mathbf{k}} \sigma_0 + \gamma_0 \boldsymbol{\gamma}_{\mathbf{k}} \cdot \boldsymbol{\sigma}, \\ \hat{\Delta}_{\mathbf{k}} &= (\Delta_s + \Delta_f \boldsymbol{\gamma}_{\mathbf{k}} \cdot \boldsymbol{\sigma})(i\sigma_y). \end{aligned} \quad (8)$$

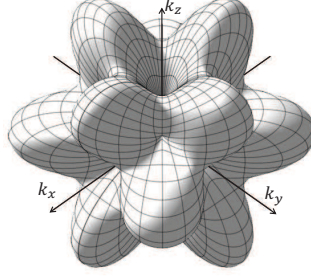


Figure 1: Schematic illustration of the amplitude of Dresselhaus SO coupling $|\gamma_{\mathbf{k}}|$ in \mathbf{k} space.

3. Nodal structures

The Bogoliubov-de Gennes quasiparticle excitation spectrum $E(\mathbf{k})$ can be obtained readily by diagonalizing the matrix $\check{H}_{\mathbf{k}}$ above. One can find four solutions, namely, $E_{\pm}^{(e)}(\mathbf{k})$ and $E_{\pm}^{(h)}(\mathbf{k})$, with $E_{\pm}^{(h)}(\mathbf{k}) = -E_{\pm}^{(e)}(\mathbf{k})$. We have

$$E_{\pm}^{(e)}(\mathbf{k}) = \sqrt{(\epsilon_{\mathbf{k}} \pm \gamma_0 |\gamma_{\mathbf{k}}|)^2 + (\Delta_s \pm \Delta_f |\gamma_{\mathbf{k}}|)^2} \equiv E_{\pm}^{\mathbf{k}}, \quad (9)$$

corresponding to two sheets of Fermi surfaces with the energy gaps given by $\Delta_{\mathbf{k}+} = \Delta_s + \Delta_f |\gamma_{\mathbf{k}}|$ and $\Delta_{\mathbf{k}-} = \Delta_s - \Delta_f |\gamma_{\mathbf{k}}|$, respectively. Zeros of $E_{\pm}^{\mathbf{k}}$ determine the nodal structure of the superconducting state in momentum space. Here let us assume a sufficiently large value of the cutoff energy ω_c ($\omega_c \gg \gamma_0, \Delta_s, \Delta_f$). It is apparent that the upper branch $E_{+}^{\mathbf{k}}$ is positive definite. Therefore, here we focus on the zeros of the lower branch $E_{-}^{\mathbf{k}}$.

The amplitude of the Dresselhaus SO coupling $|\gamma_{\mathbf{k}}|$ (see Fig. 1) becomes zero at 14 points (such as the south and north poles), possesses 24 saddle points at $(\theta_k = \arctan 2\sqrt{2}, \phi_k = \arccos \sqrt{2}/4)$, etc. with $|\gamma_{\mathbf{k}}| = 2\sqrt{2}/9$, and attains its maximum value 0.5 at 12 points $(\theta_k = \pi/2, \phi_k = \pi/4)$, etc. on the Fermi surface. Therefore, one encounters different nodal topology depending on the ratio $\kappa \equiv \Delta_s/\Delta_f$. When $\kappa = 0$ ($\kappa = 0.5$), $E_{-}^{\mathbf{k}}$ shows 14 (12) nodal points of first-order (second-order), while exhibits line nodes for $0 < \kappa < 0.5$ as displayed in Fig. 2. For $\kappa > 0.5$, however, we always have $\Delta_{\mathbf{k}-} \neq 0$, and thus the quasiparticle excitation spectrum is gapped.

4. Nuclear magnetic relaxation rate

Let us consider the temperature dependence of the nuclear magnetic relaxation rate T_1^{-1} defined as

$$\frac{1}{T_1 T} \propto \sum_{\mathbf{q}} \frac{\Im[\chi_{-+}(\mathbf{q}, i\omega_n \rightarrow \omega + i0^+)]}{\omega} \Big|_{\omega \rightarrow 0}, \quad (10)$$

where \Im denotes the imaginary part. The dynamical susceptibility in imaginary time is given by

$$\chi_{-+}(\mathbf{q}, i\omega_n) = \int_0^{1/T} d\tau \sum_{\mathbf{k}\mathbf{k}'} \left\langle \hat{T} c_{\mathbf{k}'-\mathbf{q}\downarrow}^\dagger(\tau) c_{\mathbf{k}'\uparrow}(\tau) c_{\mathbf{k}+\mathbf{q}\uparrow}^\dagger(0) c_{\mathbf{k}\downarrow}(0) \right\rangle e^{i\omega_n \tau}, \quad (11)$$

where \hat{T} denotes the time-ordering operator, $\omega_n = (2n+1)\pi T$ is the Matsubara frequency, and $c_{\mathbf{k}}(\tau) = e^{iH\tau} c_{\mathbf{k}} e^{-iH\tau}$. We obtain an explicit expression for T_1^{-1} as

$$\frac{1}{T_1 T} \propto \sum_{\mathbf{k}, \mathbf{q}} \sum_{\ell, j=\pm} \frac{\delta(E_\ell^{\mathbf{k}} - E_j^{\mathbf{q}})}{T \cosh^2(E_\ell^{\mathbf{k}}/2T)} \left(1 + \frac{\epsilon_{\ell, \mathbf{k}} \epsilon_{j, \mathbf{q}} + \Delta_{\ell, \mathbf{k}} \Delta_{j, \mathbf{q}}}{E_\ell^{\mathbf{k}} E_j^{\mathbf{q}}}\right),$$

where $\epsilon_{\pm, \mathbf{k}} = \epsilon_{\mathbf{k}} \pm \gamma_0 |\gamma_{\mathbf{k}}|$. The temperature dependence of Δ_s and Δ_f are determined by the self-consistent gap equations:

$$\begin{aligned} \Delta_s &= \sum_{\mathbf{k}, \ell} \frac{\tanh(E_\ell^{\mathbf{k}}/2T)}{4E_\ell^{\mathbf{k}}} \Delta_{\ell, \mathbf{k}} (V_s + \ell V_m |\gamma_{\mathbf{k}}|), \\ \Delta_f &= \sum_{\mathbf{k}, \ell} \frac{\tanh(E_\ell^{\mathbf{k}}/2T)}{4E_\ell^{\mathbf{k}}} \Delta_{\ell, \mathbf{k}} (V_m + \ell V_f |\gamma_{\mathbf{k}}|). \end{aligned} \quad (12)$$

It turns out that for given values of V_s, V_f , and ω_c , $1/T_1 T$ depends on the Δ_s and Δ_f only through the ratio κ , and is independent of the strength of SO coupling γ_0 , similar to the case of Ref. [13]. It is interesting to see how the low-temperature power law behaviour for the nuclear spin-lattice relaxation rate $1/T_1 T \propto T^n$ is changed with the ratio κ . Plotted in Fig. 3 is the exponent of temperature, n , as a function of κ at $T = 0.04T_c$ calculated numerically according to $n = d \ln(1/T_1 T) / d \ln T$ [23]. As we see, the exponent n attains its maximum $n = 4$ at $\kappa = 0$ (point node of first-order), decreases oscillatorily

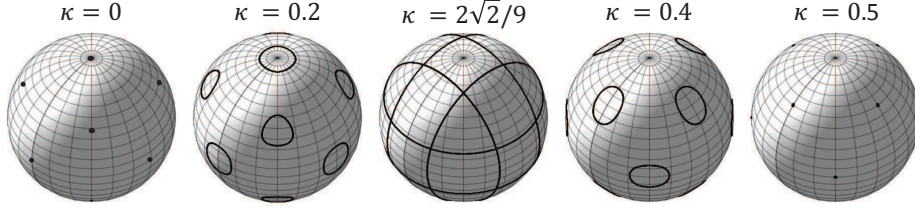


Figure 2: Evolution of nodal structure with the parameter κ ($0 \leq \kappa \leq 0.5$). At $\kappa = 0$ ($\kappa = 0.5$), $E_-^{\mathbf{k}}$ shows 14 (12) nodal points of first-order (second-order), while exhibits line nodes for $0 < \kappa < 0.5$.

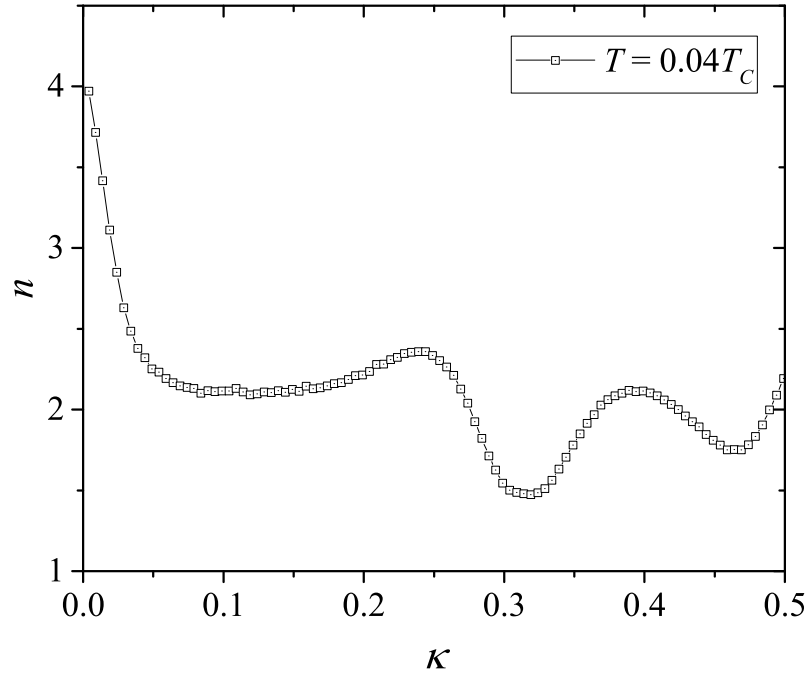


Figure 3: The exponent of temperature as a function of κ , calculated numerically according to $n = d \ln(1/T_1 T) / d \ln T$.

with increasing κ , and end with $n \approx 2.2$ at $\kappa = 0.5$. It is worth noting that, the exponent n is not necessarily to be an integer here, similar to the cases in Ref. [23]. For $\kappa > 0.5$, however, the gap is open and $1/T_1T$ decays exponentially in nature. We present in Fig. 4 the temperature dependence of $1/T_1T$ obtained experimentally [18] by Harada *et al.* for Y_2C_3 , together with the calculated results for $\kappa=0.47$, 0.50, and 0.53 for comparison. Shown in the inset of Fig. 4 is the detailed temperature dependence of Δ_s and Δ_f obtained by solving the gap equations Eq. (12) for $\kappa = 0.53$. As can be seen from Fig. 4, there is a fair agreement between our simple theory and experimental results. However, further experimental measurements at low temperatures $T/T_c < 0.15$ are needed to obtain a decisive information about the pairing symmetry and to test the prediction of our theory.

5. Summary

In summary, we have calculated the temperature dependence of the nuclear magnetic relaxation rate $1/T_1T$ in the Dresselhaus-type noncentrosymmetric superconductor Y_2C_3 . We have considered the $(s+f)$ -wave parity-mixing model where the d -vector is chosen to be parallel to the Dresselhaus SO coupling vector. It is found that various types of nodal structures can be generated due to the effect of parity-mixing, depending on the value of κ . We also find that, for $\kappa \sim 0.5$, the $(s+f)$ -wave model can explain the experimental results fairly well over a wide range of temperatures. However, accurate measurements of $1/T_1T$ at lower temperatures would be crucial to the further clarification of pairing symmetry and gap structure in Y_2C_3 .

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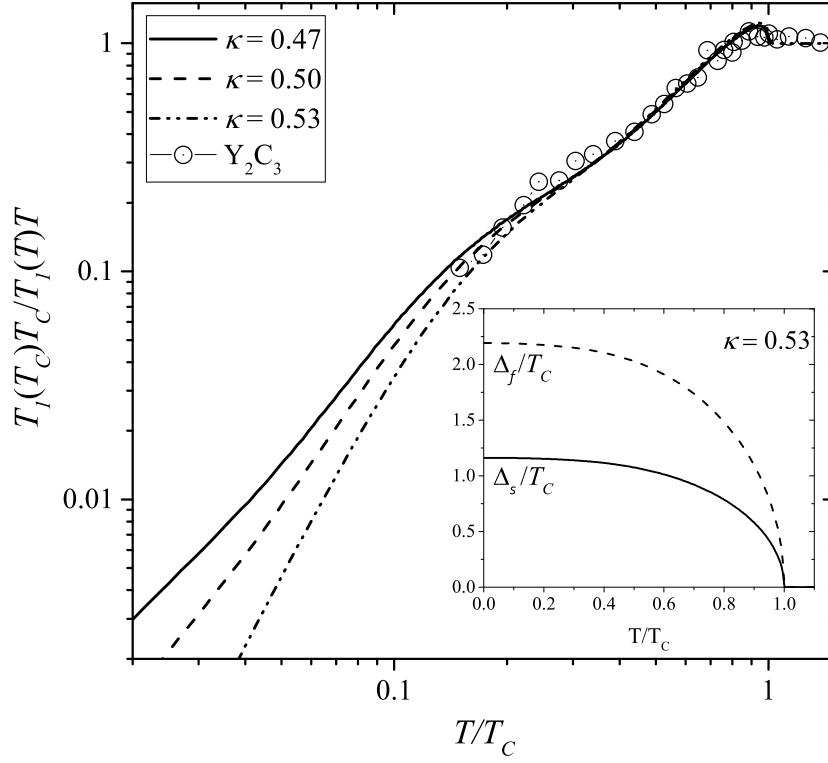


Figure 4: Comparison of the experimental data in Ref. [18] with the calculated temperature dependence of $1/T_1 T$ for $\kappa = 0.47, 0.5$, and 0.53 . Inset shows the temperature dependence of Δ_s and Δ_f at $\kappa = 0.53$.

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